



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2017 – 06:51 PM EST

PDB ID : 4L1B  
Title : Crystal Structure of p110alpha complexed with niSH2 of p85alpha  
Authors : Zhang, J.; Zhao, Y.L.; Chen, Y.Y.; Huang, M.; Jiang, F.  
Deposited on : unknown  
Resolution : 2.59 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

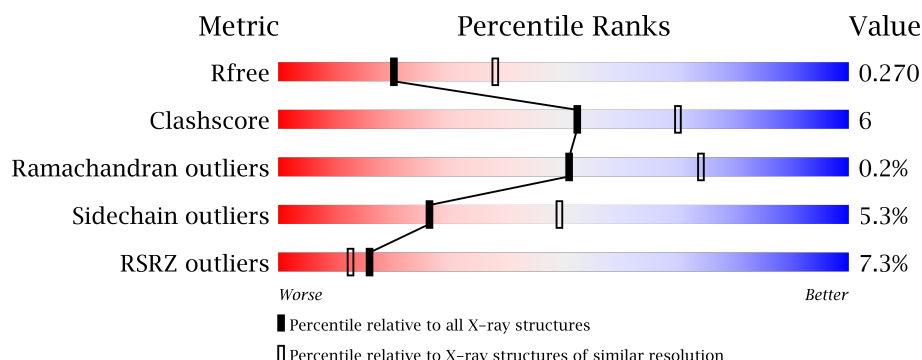
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2899 (2.60-2.56)
Clashscore	112137	3268 (2.60-2.56)
Ramachandran outliers	110173	3218 (2.60-2.56)
Sidechain outliers	110143	3218 (2.60-2.56)
RSRZ outliers	101464	2907 (2.60-2.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1068	<div> <div>7%</div> <div>75%</div> <div>17%</div> <div>• 7%</div> </div>
2	B	324	<div> <div>7%</div> <div>67%</div> <div>16%</div> <div>• 15%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10528 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			8132	5205	1383	1476	68			

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	277	Total	C	N	O	S	0	0	0
			2354	1474	420	452	8			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	292	MET	-	EXPRESSION TAG	UNP P27986
B	293	SER	-	EXPRESSION TAG	UNP P27986
B	294	TYR	-	EXPRESSION TAG	UNP P27986
B	295	TYR	-	EXPRESSION TAG	UNP P27986
B	296	HIS	-	EXPRESSION TAG	UNP P27986
B	297	HIS	-	EXPRESSION TAG	UNP P27986
B	298	HIS	-	EXPRESSION TAG	UNP P27986
B	299	HIS	-	EXPRESSION TAG	UNP P27986
B	300	HIS	-	EXPRESSION TAG	UNP P27986
B	301	HIS	-	EXPRESSION TAG	UNP P27986
B	302	ASP	-	EXPRESSION TAG	UNP P27986
B	303	TYR	-	EXPRESSION TAG	UNP P27986
B	304	ASP	-	EXPRESSION TAG	UNP P27986
B	305	ILE	-	EXPRESSION TAG	UNP P27986
B	306	PRO	-	EXPRESSION TAG	UNP P27986
B	307	THR	-	EXPRESSION TAG	UNP P27986
B	308	THR	-	EXPRESSION TAG	UNP P27986
B	309	GLU	-	EXPRESSION TAG	UNP P27986
B	310	ASN	-	EXPRESSION TAG	UNP P27986

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	311	LEU	-	EXPRESSION TAG	UNP P27986
B	312	TYR	-	EXPRESSION TAG	UNP P27986
B	313	PHE	-	EXPRESSION TAG	UNP P27986
B	314	GLN	-	EXPRESSION TAG	UNP P27986
B	315	SER	-	EXPRESSION TAG	UNP P27986
B	316	ILE	-	EXPRESSION TAG	UNP P27986
B	317	ALA	-	EXPRESSION TAG	UNP P27986

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

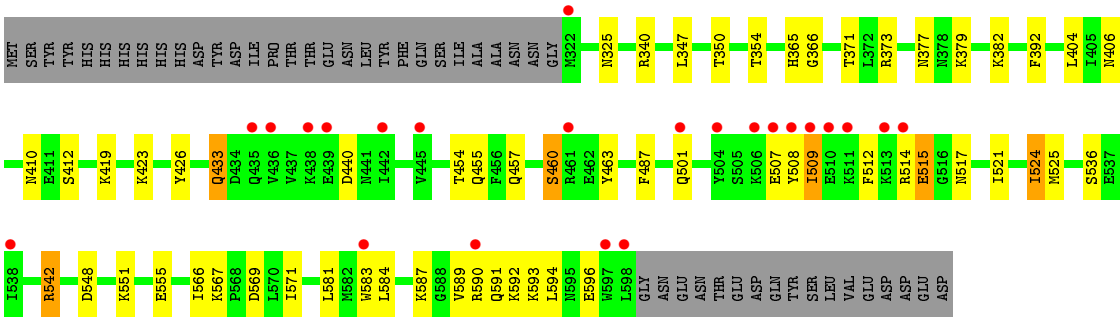


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		
4	B	6	Total	O	0	0
			6	6		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.56Å 136.90Å 150.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.09 – 2.59 47.09 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.09-2.59) 95.4 (47.09-2.59)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.217 , 0.274 0.207 , 0.270	Depositor DCC
$R_{free}$ test set	2217 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.9	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10528	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/8316	0.46	0/11242
2	B	0.25	0/2394	0.47	0/3207
All	All	0.25	0/10710	0.46	0/14449

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8132	0	8110	104	0
2	B	2354	0	2330	31	0
3	B	5	0	0	0	0
4	A	31	0	0	0	0
4	B	6	0	0	0	0
All	All	10528	0	10440	132	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (132) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:VAL:HG12	1:A:218:GLU:H	1.50	0.76
1:A:917:HIS:H	1:A:920:ASN:HB2	1.55	0.71
2:B:514:ARG:O	2:B:515:GLU:HB3	1.92	0.68
2:B:542:ARG:HH11	2:B:542:ARG:HG2	1.57	0.68
1:A:215:CYS:HB3	1:A:219:GLN:HG3	1.77	0.67
1:A:209:LEU:HD21	1:A:223:GLU:HB3	1.78	0.66
1:A:42:LEU:HD12	1:A:85:GLU:HA	1.78	0.66
1:A:537:ARG:NH1	1:A:543:ILE:HA	2.12	0.65
2:B:512:PHE:HB3	2:B:517:ASN:HB3	1.81	0.62
1:A:410:LYS:NZ	2:B:569:ASP:OD1	2.32	0.62
2:B:366:GLY:HA3	2:B:382:LYS:HD3	1.84	0.60
1:A:537:ARG:O	1:A:567:LYS:NZ	2.33	0.60
1:A:637:GLN:NE2	1:A:674:GLU:OE2	2.27	0.58
1:A:916:ARG:HB3	1:A:921:ILE:HD11	1.85	0.58
1:A:594:LYS:HG3	1:A:595:PRO:HD2	1.85	0.57
1:A:121:ILE:HG22	1:A:123:MET:HG2	1.86	0.57
1:A:537:ARG:NH1	1:A:547:GLU:OE1	2.38	0.57
1:A:1044:ASN:HA	1:A:1051:TRP:HB3	1.88	0.56
1:A:937:PHE:HD1	1:A:938:LEU:HG	1.69	0.56
2:B:507:GLU:HG3	2:B:508:TYR:HD1	1.70	0.56
1:A:68:TYR:HB3	1:A:101:VAL:HG23	1.88	0.56
2:B:509:ILE:HD11	2:B:524:ILE:HG21	1.87	0.55
1:A:1039:PHE:CZ	1:A:1043:MET:HE2	2.41	0.55
1:A:895:ASP:OD2	1:A:899:ARG:NH2	2.41	0.54
2:B:542:ARG:NH1	2:B:542:ARG:HG2	2.19	0.54
2:B:392:PHE:CZ	2:B:404:LEU:HD21	2.42	0.54
1:A:69:ILE:HG12	1:A:70:PHE:H	1.72	0.54
1:A:105:VAL:O	1:A:111:LYS:NZ	2.39	0.54
2:B:406:ASN:O	2:B:410:ASN:ND2	2.41	0.53
1:A:596:GLU:HA	1:A:599:MET:HE2	1.90	0.53
2:B:590:ARG:NE	2:B:592:LYS:HB2	2.25	0.52
2:B:433:GLN:HG3	2:B:583:TRP:HD1	1.75	0.51
1:A:199:SER:OG	1:A:201:ASN:ND2	2.43	0.51
1:A:807:LEU:HD12	1:A:846:GLY:HA3	1.93	0.51
1:A:717:ASP:O	1:A:721:GLN:HG2	2.11	0.51
1:A:129:ASP:OD1	1:A:140:ARG:NH1	2.43	0.50
1:A:194:ILE:HD13	1:A:209:LEU:HD22	1.93	0.50
2:B:463:TYR:HB2	2:B:566:ILE:HG21	1.93	0.50
1:A:121:ILE:HD12	1:A:688:LEU:HB3	1.93	0.50
1:A:640:LYS:HG2	1:A:680:VAL:HG11	1.93	0.50
1:A:959:ASP:O	1:A:963:VAL:HG23	2.12	0.50
1:A:135:GLU:HG2	1:A:645:LEU:HD12	1.93	0.49

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ILE:HG21	1:A:551:LEU:HD11	1.94	0.49
1:A:305:PRO:HB3	1:A:693:ARG:NH1	2.28	0.49
1:A:947:TYR:HD1	1:A:949:ARG:HB3	1.78	0.48
1:A:69:ILE:HG12	1:A:70:PHE:N	2.28	0.48
2:B:551:LYS:O	2:B:555:GLU:HG3	2.13	0.48
1:A:1031:THR:HG23	1:A:1033:GLN:H	1.79	0.48
2:B:365:HIS:O	2:B:382:LYS:HD3	2.14	0.48
2:B:567:LYS:O	2:B:571:ILE:HG12	2.13	0.48
1:A:819:ILE:O	1:A:823:ILE:HG12	2.13	0.47
1:A:883:ASP:HA	1:A:886:LYS:HD3	1.96	0.47
1:A:133:ASP:HA	1:A:134:PRO:HD2	1.78	0.47
1:A:787:ASP:O	1:A:790:SER:HB2	2.15	0.47
1:A:542:GLU:OE1	2:B:340:ARG:HD3	2.15	0.47
1:A:728:GLN:HB2	1:A:729:LYS:HE3	1.97	0.47
2:B:584:LEU:HD22	2:B:589:VAL:HG21	1.97	0.46
2:B:591:GLN:HA	2:B:594:LEU:HD12	1.98	0.46
1:A:9:GLU:OE2	1:A:16:MET:HG2	2.15	0.46
1:A:189:GLN:HG2	1:A:212:ASN:HA	1.97	0.46
1:A:72:SER:OG	1:A:73:VAL:N	2.47	0.46
1:A:917:HIS:CE1	1:A:919:SER:HB2	2.51	0.45
2:B:350:THR:OG1	2:B:373:ARG:HG3	2.16	0.45
2:B:347:LEU:HD22	2:B:373:ARG:HG2	1.99	0.45
1:A:195:TRP:CE3	1:A:204:LYS:HB2	2.51	0.45
1:A:282:MET:HA	1:A:283:PRO:HD2	1.82	0.45
1:A:969:GLN:H	1:A:969:GLN:CD	2.19	0.45
2:B:512:PHE:HB2	2:B:521:ILE:HD11	1.98	0.45
1:A:26:LEU:HD23	1:A:101:VAL:HG11	1.98	0.45
1:A:529:GLU:HA	1:A:532:LYS:HE2	1.97	0.45
1:A:942:LYS:HD2	1:A:947:TYR:O	2.17	0.45
1:A:833:MET:HE1	1:A:903:GLY:HA3	1.99	0.45
1:A:619:LEU:HD22	1:A:623:LEU:HD22	1.99	0.44
1:A:1044:ASN:ND2	1:A:1051:TRP:O	2.45	0.44
1:A:199:SER:HB2	1:A:200:PRO:HD2	1.99	0.44
1:A:1054:LYS:HA	1:A:1054:LYS:HD2	1.79	0.44
1:A:46:LYS:HG2	1:A:65:GLU:HB3	1.99	0.44
1:A:934:PHE:O	1:A:936:HIS:N	2.50	0.44
1:A:1024:LYS:HB2	1:A:1024:LYS:HE3	1.66	0.44
1:A:1053:THR:HB	1:A:1055:MET:H	1.83	0.44
2:B:371:THR:HA	2:B:379:LYS:O	2.17	0.44
1:A:600:GLU:HB2	1:A:1000:ASN:ND2	2.33	0.44
1:A:121:ILE:HD11	1:A:692:CYS:SG	2.58	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:MET:HA	1:A:492:ILE:HD12	1.98	0.44
1:A:148:LYS:HE2	1:A:148:LYS:HB3	1.59	0.43
1:A:947:TYR:CD1	1:A:949:ARG:HB3	2.53	0.43
1:A:1031:THR:HG22	1:A:1034:GLU:H	1.82	0.43
1:A:54:ARG:HA	1:A:59:HIS:CD2	2.52	0.43
1:A:121:ILE:CD1	1:A:688:LEU:HB3	2.48	0.43
1:A:357:ARG:NH2	1:A:370:ASN:HD22	2.17	0.43
1:A:521:ASN:HB2	1:A:557:TYR:OH	2.19	0.43
1:A:360:ILE:HG22	1:A:367:LEU:HD12	2.00	0.43
1:A:940:HIS:C	1:A:942:LYS:H	2.21	0.43
1:A:365:GLU:HG3	2:B:377:ASN:OD1	2.18	0.43
2:B:457:GLN:HA	2:B:460:SER:HB2	2.00	0.43
1:A:479:TRP:CZ3	1:A:481:SER:HA	2.53	0.43
2:B:412:SER:HA	2:B:423:LYS:HG2	2.01	0.42
1:A:613:GLY:HA2	1:A:648:LEU:HD12	2.00	0.42
1:A:917:HIS:HE1	1:A:919:SER:HB2	1.84	0.42
1:A:727:THR:HB	1:A:729:LYS:HD2	2.02	0.42
2:B:590:ARG:HB3	2:B:593:LYS:HG3	2.01	0.42
1:A:220:VAL:HB	1:A:252:LEU:HD11	2.02	0.42
1:A:180:HIS:ND1	1:A:828:GLY:HA2	2.35	0.42
1:A:297:LEU:HA	1:A:298:PRO:HD3	1.68	0.42
1:A:27:PRO:HG3	1:A:101:VAL:O	2.20	0.42
1:A:404:LEU:HD11	1:A:443:LEU:HD23	2.01	0.42
1:A:468:LYS:HD3	1:A:468:LYS:HA	1.93	0.42
1:A:216:VAL:O	1:A:219:GLN:HG2	2.20	0.41
1:A:702:LEU:HD23	1:A:702:LEU:HA	1.88	0.41
1:A:776:LYS:HD2	1:A:804:GLY:HA3	2.03	0.41
2:B:382:LYS:HE3	2:B:382:LYS:HB2	1.92	0.41
1:A:532:LYS:O	1:A:536:THR:HG23	2.20	0.41
1:A:1048:HIS:C	1:A:1050:GLY:H	2.24	0.41
1:A:429:LEU:HA	1:A:429:LEU:HD23	1.83	0.41
1:A:140:ARG:HD3	1:A:689:GLU:OE1	2.21	0.41
1:A:755:LEU:HD23	1:A:755:LEU:HA	1.95	0.41
2:B:354:THR:HA	2:B:426:TYR:O	2.21	0.41
1:A:676:HIS:CD2	1:A:843:ASP:HB2	2.56	0.41
2:B:583:TRP:CH2	2:B:587:LYS:HE2	2.56	0.41
1:A:181:ILE:HD12	1:A:278:MET:SD	2.61	0.40
1:A:187:LYS:HE3	1:A:187:LYS:HB2	1.83	0.40
1:A:223:GLU:O	1:A:226:ARG:HG2	2.21	0.40
1:A:357:ARG:HH21	1:A:370:ASN:HD22	1.70	0.40
2:B:593:LYS:O	2:B:596:GLU:HG2	2.21	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLU:HB2	1:A:88:ARG:HE	1.86	0.40
1:A:42:LEU:HD11	1:A:82:PHE:HB3	2.03	0.40
1:A:834:LEU:HD12	1:A:834:LEU:HA	1.82	0.40
1:A:904:TYR:CE1	1:A:930:PHE:HA	2.56	0.40
1:A:151:VAL:HG12	1:A:154:ARG:NH2	2.37	0.40
1:A:178:PRO:HB2	1:A:181:ILE:HG12	2.04	0.40
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.57	0.40
1:A:857:ILE:HA	1:A:857:ILE:HD13	1.90	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	982/1068 (92%)	932 (95%)	48 (5%)	2 (0%)	51	74
2	B	275/324 (85%)	266 (97%)	8 (3%)	1 (0%)	38	61
All	All	1257/1392 (90%)	1198 (95%)	56 (4%)	3 (0%)	51	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	935	GLY
2	B	515	GLU
1	A	264	LYS

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	910/974 (93%)	864 (95%)	46 (5%)	28	51
2	B	258/301 (86%)	242 (94%)	16 (6%)	21	41
All	All	1168/1275 (92%)	1106 (95%)	62 (5%)	26	49

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ILE
1	A	60	GLN
1	A	89	LEU
1	A	93	ARG
1	A	101	VAL
1	A	109	GLU
1	A	115	ARG
1	A	121	ILE
1	A	140	ARG
1	A	162	ARG
1	A	187	LYS
1	A	197	ILE
1	A	219	GLN
1	A	223	GLU
1	A	225	ILE
1	A	281	ARG
1	A	292	SER
1	A	301	CYS
1	A	329	VAL
1	A	358	THR
1	A	369	ASP
1	A	378	CYS
1	A	475	LEU
1	A	488	ASP
1	A	490	SER
1	A	576	SER
1	A	626	ASP
1	A	681	SER
1	A	682	GLN
1	A	687	LEU
1	A	700	LYS
1	A	729	LYS
1	A	774	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	784	GLU
1	A	788	ILE
1	A	862	CYS
1	A	875	HIS
1	A	883	ASP
1	A	901	CYS
1	A	942	LYS
1	A	945	PHE
1	A	947	TYR
1	A	959	ASP
1	A	974	THR
1	A	1031	THR
1	A	1053	THR
2	B	325	ASN
2	B	419	LYS
2	B	433	GLN
2	B	440	ASP
2	B	454	THR
2	B	455	GLN
2	B	460	SER
2	B	487	PHE
2	B	501	GLN
2	B	509	ILE
2	B	524	ILE
2	B	525	MET
2	B	536	SER
2	B	542	ARG
2	B	548	ASP
2	B	581	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	60	GLN
1	A	201	ASN
1	A	370	ASN
1	A	444	ASN
1	A	795	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	B	701	-	4,4,4	0.17	0	6,6,6	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	B	701	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	994/1068 (93%)	0.55	70 (7%) 17 14	38, 63, 109, 164	0
2	B	277/324 (85%)	0.49	23 (8%) 12 9	45, 70, 123, 135	0
All	All	1271/1392 (91%)	0.54	93 (7%) 16 13	38, 65, 114, 164	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	LEU	7.9
1	A	243	VAL	6.1
1	A	202	ASN	6.0
1	A	197	ILE	4.8
1	A	1055	MET	4.8
1	A	156	LEU	4.7
1	A	947	TYR	4.7
1	A	298	PRO	4.5
2	B	507	GLU	4.4
1	A	221	ILE	4.3
1	A	945	PHE	4.0
1	A	1057	TRP	4.0
2	B	509	ILE	3.8
1	A	481	SER	3.8
2	B	435	GLN	3.8
1	A	70	PHE	3.8
2	B	508	TYR	3.6
1	A	414	GLY	3.6
1	A	323	SER	3.5
2	B	438	LYS	3.4
2	B	510	GLU	3.3
1	A	295	SER	3.2
1	A	793	LEU	3.1
2	B	598	LEU	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	1054	LYS	3.0
2	B	442	ILE	3.0
1	A	186	ASP	3.0
1	A	207	TYR	2.9
1	A	297	LEU	2.9
1	A	944	LYS	2.9
1	A	792	LEU	2.9
1	A	13	ILE	2.8
1	A	62	LEU	2.8
2	B	322	MET	2.8
1	A	220	VAL	2.7
1	A	285	LEU	2.7
2	B	513	LYS	2.7
1	A	293	LEU	2.7
2	B	597	TRP	2.7
1	A	1046	ALA	2.7
2	B	436	VAL	2.6
1	A	671	LEU	2.6
1	A	245	GLU	2.6
1	A	61	LEU	2.6
2	B	511	LYS	2.6
1	A	200	PRO	2.5
1	A	86	THR	2.5
1	A	722	GLU	2.5
1	A	1058	ILE	2.5
1	A	49	LEU	2.4
1	A	209	LEU	2.4
1	A	194	ILE	2.4
2	B	583	TRP	2.4
2	B	439	GLU	2.3
1	A	267	LEU	2.3
1	A	500	VAL	2.3
2	B	590	ARG	2.3
1	A	211	ILE	2.3
1	A	250	TYR	2.3
1	A	306	SER	2.3
1	A	226	ARG	2.3
1	A	299	MET	2.3
2	B	445	VAL	2.3
1	A	633	ILE	2.3
1	A	744	PHE	2.3
1	A	205	GLN	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	37	LEU	2.2
2	B	506	LYS	2.2
1	A	43	ILE	2.2
1	A	881	LEU	2.2
1	A	68	TYR	2.2
1	A	246	TYR	2.2
1	A	499	SER	2.1
2	B	514	ARG	2.1
1	A	196	VAL	2.1
2	B	504	TYR	2.1
2	B	501	GLN	2.1
1	A	524	ARG	2.1
1	A	45	ILE	2.1
1	A	888	GLU	2.1
1	A	861	GLN	2.1
1	A	307	TYR	2.1
1	A	15	LEU	2.1
1	A	180	HIS	2.1
1	A	875	HIS	2.1
1	A	599	MET	2.1
1	A	943	LYS	2.1
2	B	461	ARG	2.1
1	A	294	TYR	2.0
1	A	320	GLY	2.0
2	B	538	ILE	2.0
1	A	638	VAL	2.0
1	A	179	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	B	701	5/5	0.97	0.13	-0.68	63,66,68,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.